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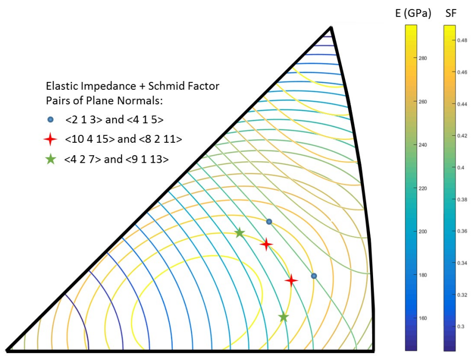
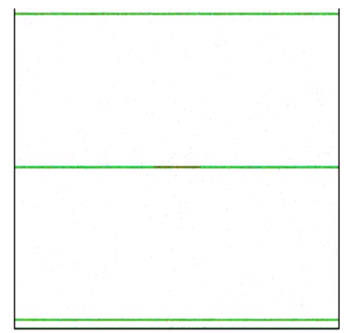
A primer on selecting grain boundary sets for comparison of interfacial fracture properties in MD simulations





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2017 LAMMPS Workshop & Symposium

August 1st - August 3rd, Albuquerque NM

U.S. DEPARTMENT OF ENERGY · NNSA National Nuclear Security Administration · LDRD Laboratory Directed Research & Development

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LAMMPS random fact of the day:

Fast parallel algorithms for short-range molecular dynamics
S Plimpton - Journal of computational physics, 1995 - Elsevier
Three parallel algorithms for classical molecular dynamics are presented. The first assigns each processor a fixed subset of atoms; the second assigns each a fixed subset of inter-atomic forces to compute; the third assigns each a fixed spatial region. The algorithms are
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crack

About 1,590 results (0.03 sec)

interfacial crack

About 563 results (0.07 sec)

Fast parallel algorithms for short-range molecular dynamics

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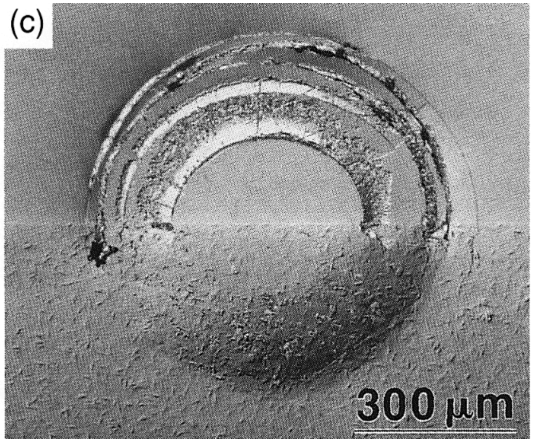
[Source: Google scholar as a 8/3/2017]

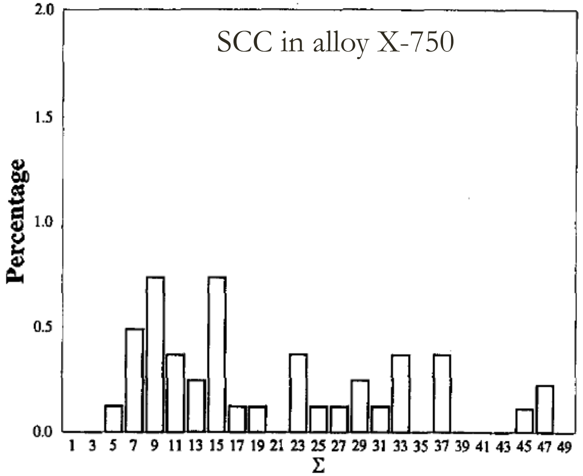
Fundamentals of fracture processes influenced by interfacial structure

Crack resistant glass/ceramic



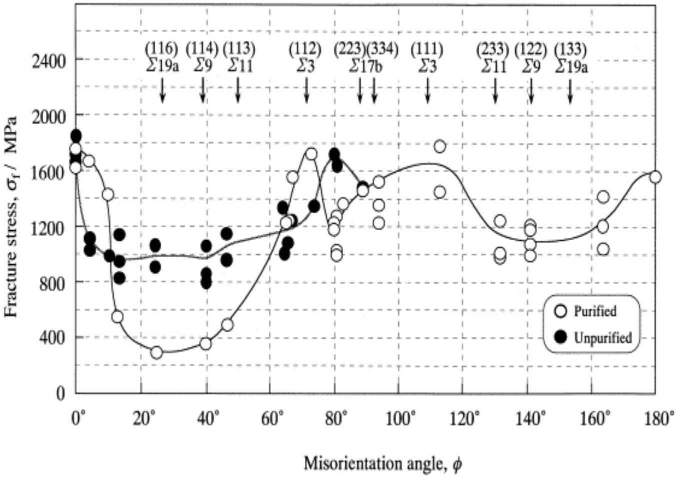
[Wuttiphan, 1996, JAmCeramSoc]

GB effects on intergranular SCC



[Pan, 1996, ActaMater]

Fracture stress in Mo bicrystals



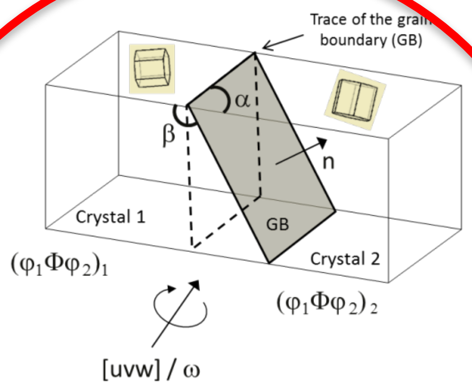
[Watanabe, 1999, ActaMater]

- **Interfacial attributes of importance:**
  - Elastic mismatch
  - Degree of symmetry
  - Interfacial coherency (structure)
    (physical and the chemical nature between both phases)

$$\sigma(r,\theta) = \frac{\mathfrak{Re}\left(Kr^{i\epsilon}\right)}{\sqrt{2\pi r}}\hat{\sigma}^{I}(\theta) + \frac{\mathfrak{Im}\left(Kr^{i\epsilon}\right)}{\sqrt{2\pi r}}\hat{\sigma}^{II}(\theta) + \frac{K_{III}}{\sqrt{2\pi r}}\hat{\sigma}^{III}(\theta)$$

$$\epsilon = \frac{1}{2\pi}\ln\left(\frac{1-\beta}{1+\beta}\right) \quad , \quad \beta = \frac{\mu_1(k_2-1)-\mu_2(k_1-1)}{\mu_1(k_2+1)+\mu_2(k_1+1)}$$

How do we isolate (decouple) the role of the interface structure on interfacial fracture?



Misorientation space

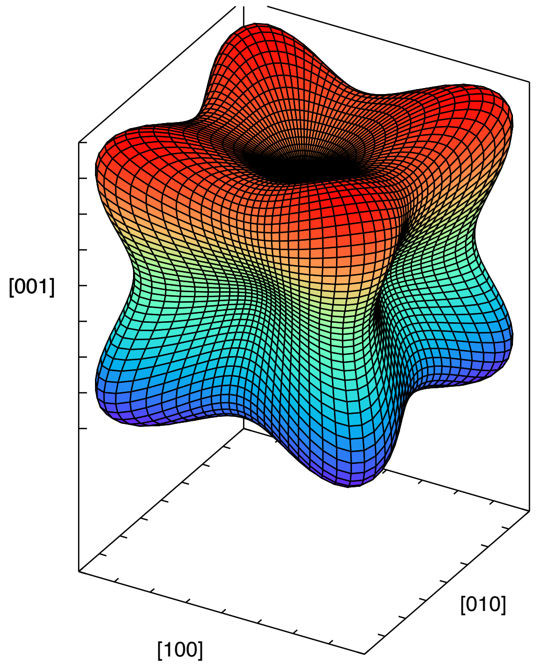
$$\sigma\left(r,\theta\right)=\frac{\mathfrak{Re}\left(Kr^{i\epsilon}\right)}{\sqrt{2\pi r}}\hat{\sigma}^{\mathrm{I}}\left(\theta\right)+\frac{\mathfrak{Im}\left(Kr^{i\epsilon}\right)}{\sqrt{2\pi r}}\hat{\sigma}^{\mathrm{II}}\left(\theta\right)+\frac{K_{\mathrm{III}}}{\sqrt{2\pi r}}\hat{\sigma}^{\mathrm{III}}\left(\theta\right)$$

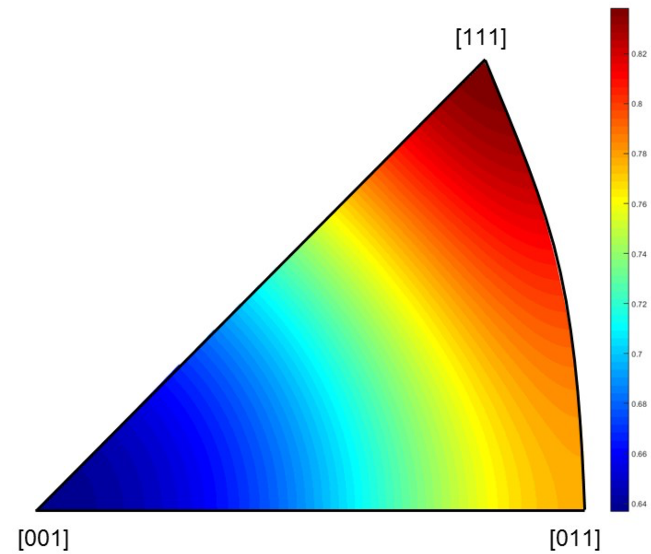
$$\epsilon=\frac{1}{2\pi}\ln\left(\frac{1-\beta}{1+\beta}\right)\quad,\quad\beta=\frac{\mu_1\left(k_2-1\right)-\mu_2\left(k_1-1\right)}{\mu_1\left(k_2+1\right)+\mu_2\left(k_1+1\right)}$$

Fracture properties space

- **Create grain boundaries with matching important fracture-related properties of adjoining lattices:**
  - Anisotropic elastic moduli
  - Schmid factor
  - Slip mode

Criterion: Elastic Anisotropy



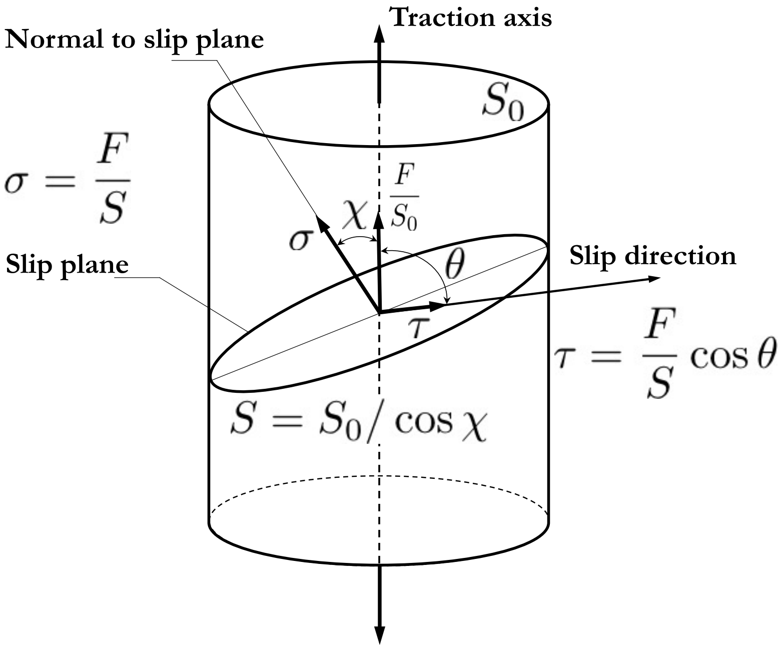


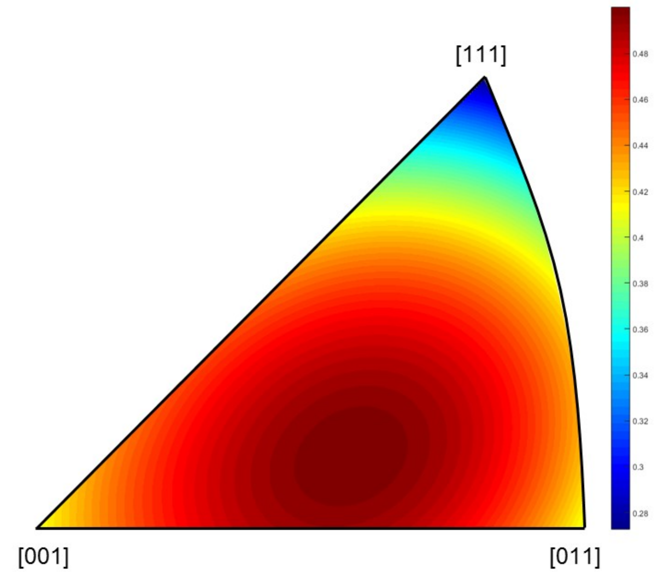
- **Orientation dependent Young's modulus:**

$$\frac{1}{E_{\overrightarrow{X}}} = \frac{\mathbb{C}_{11} + \mathbb{C}_{12}}{\left(\mathbb{C}_{11} - \mathbb{C}_{12}\right)\left(\mathbb{C}_{11} + 2\mathbb{C}_{12}\right)} + \left(\frac{1}{\mathbb{C}_{44}} - 2\frac{1}{\mathbb{C}_{11} - \mathbb{C}_{12}}\right)\frac{x_1^2 x_2^2 + x_2^2 x_3^2 + x_1^2 x_3^2}{||\overrightarrow{X}||^4}$$

  - Difference in elastic anisotropy lead to localization effects at GB but also a contributing factor for SIF (Dundur's parameters)

Criterion: Schmid factor for primary slip



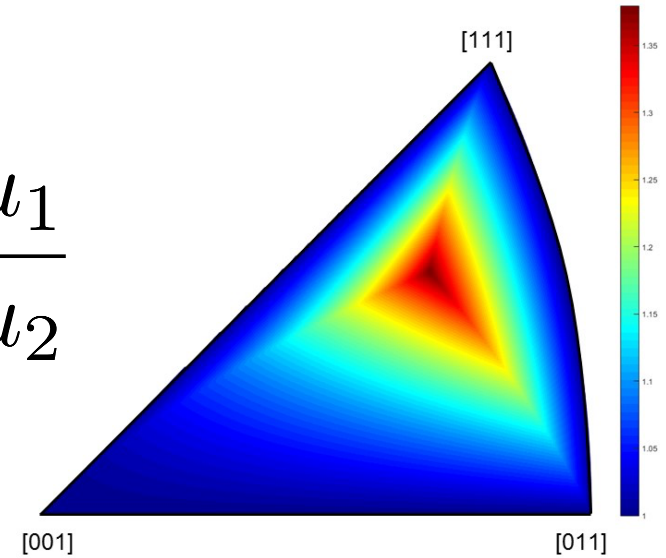


$$\tau^\alpha = \mu^\alpha \cdot \sigma \ , \text{with } \mu^\alpha = \cos\chi \cos\theta$$

- Largest resolved shear stress on any slip system defines the primary slip system to be activated upon plasticity activity.

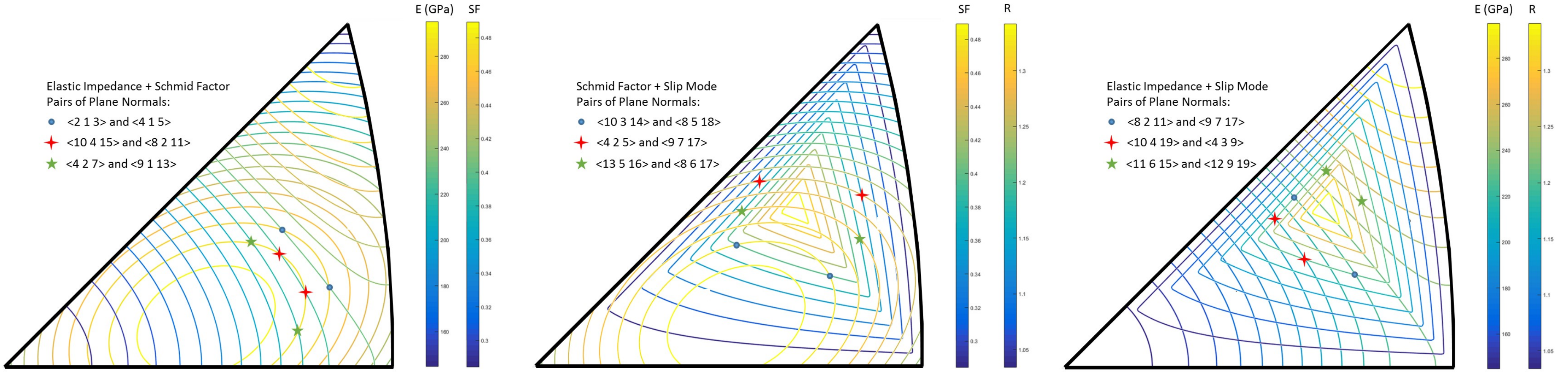
Criterion: Slide mode

$$\mu^{\alpha} = \begin{bmatrix} \mu^1 \\ \mu^2 \\ \mu^3 \\ . \\ . \\ \mu^n \end{bmatrix} \qquad R_{\mu} = \frac{\mu_1}{\mu_2}$$



- Slip mode and potential for second slip system to be activated with respect to first activated slip system:
  - Single versus multi-slip

Eliminating role of selected lattice attributes in comparative analysis of interfacial fracture:

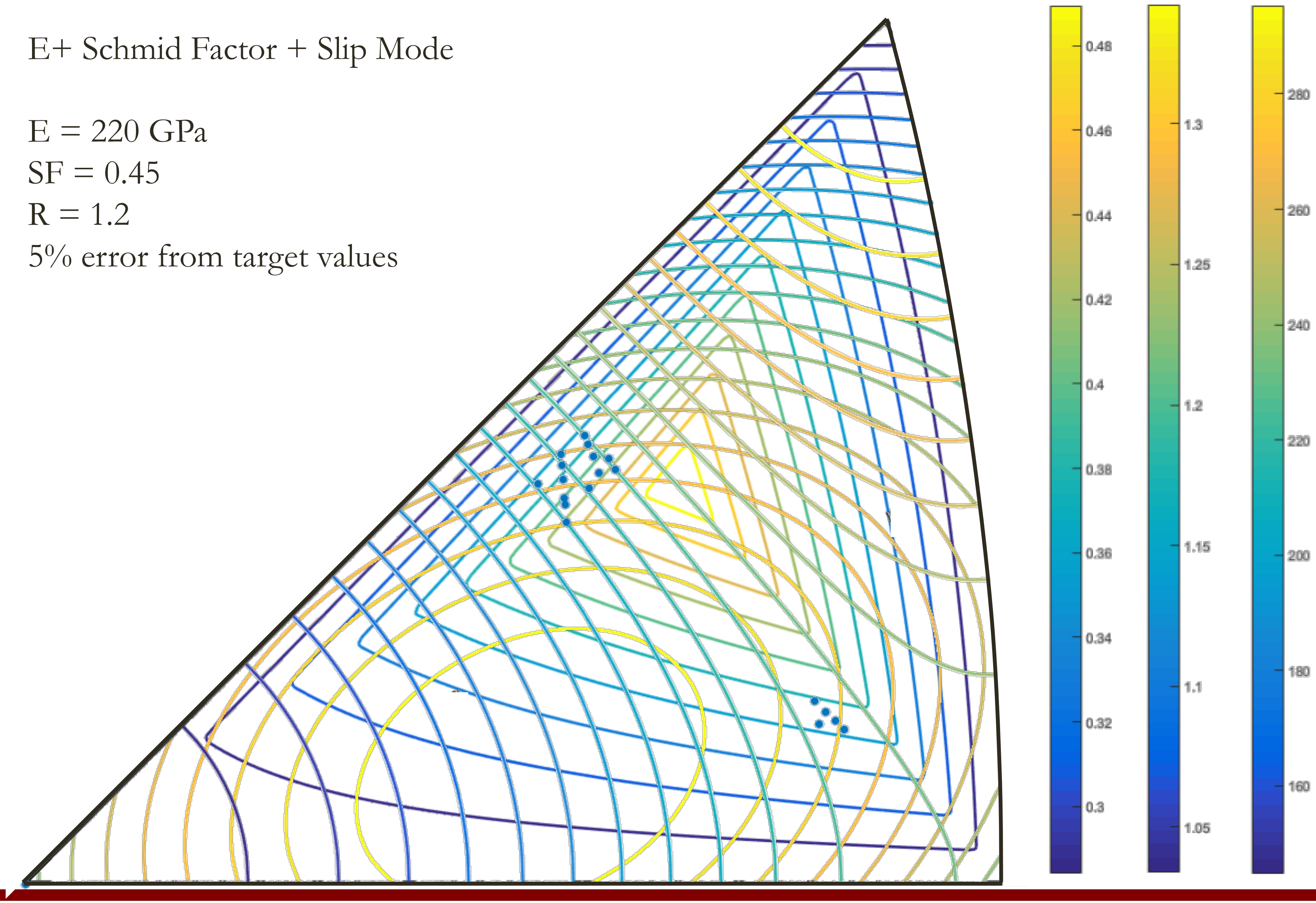


- **Matching of lattice attributes:**
  - Directional Young's modulus and Schmid factor for primary slip
    - Importance of elastic/plastic transition
  - Directional Young's modulus and slip mode
    - Importance of partitioning of dislocation activities
  - Schmid factor for primary slip and slip mode
    - Importance of elastic anisotropy/elastic impedance

Grouping orientations

E+ Schmid Factor + Slip Mode

E = 220 GPa
SF = 0.45
R = 1.2
5% error from target values



Case study

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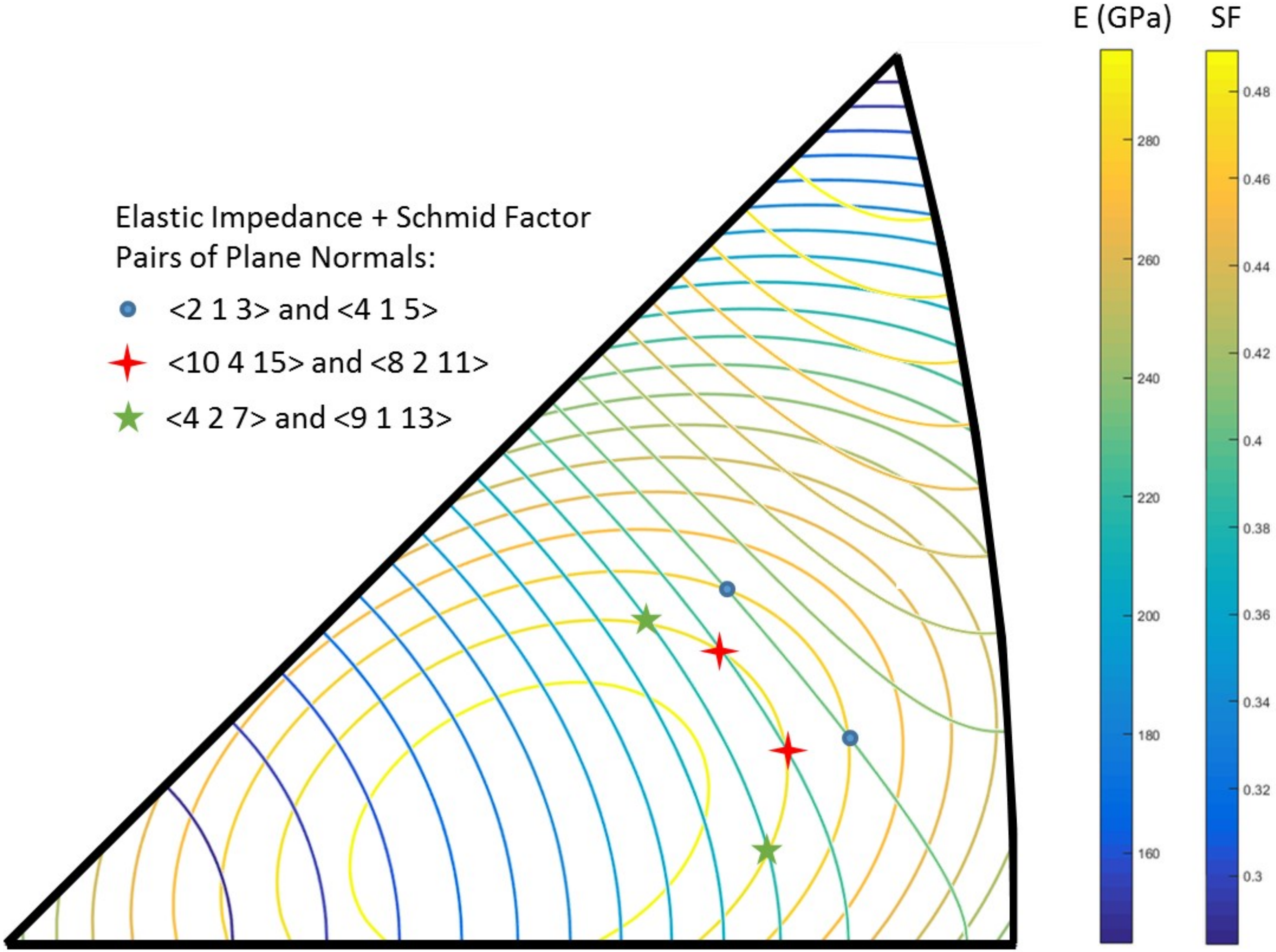

Simulating steady-state fracture

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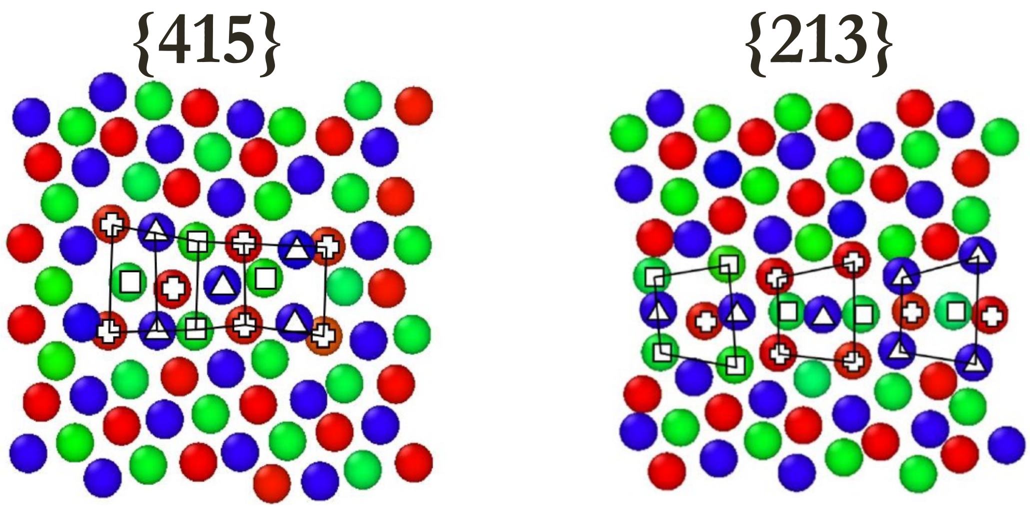
Step 1
Build grain boundary structure

Step 2
Equilibrate system under pre-tension

Step 3
Introduce atomically sharp crack

Step 4
Allow crack growth under pre-tension

Step 5
Averaging to extract decohesion form



GB Normal	GB CSL	$E_{\vec{X}}$ [GPa]	μ	R_μ
⟨2 1 3⟩	Σ21	232.6	0.467	1.33
⟨4 1 5⟩	Σ7	232.6	0.467	1.20

[Yamakov et al., 2006, JMPS]
[Barrows et al., 2016, MSEA]

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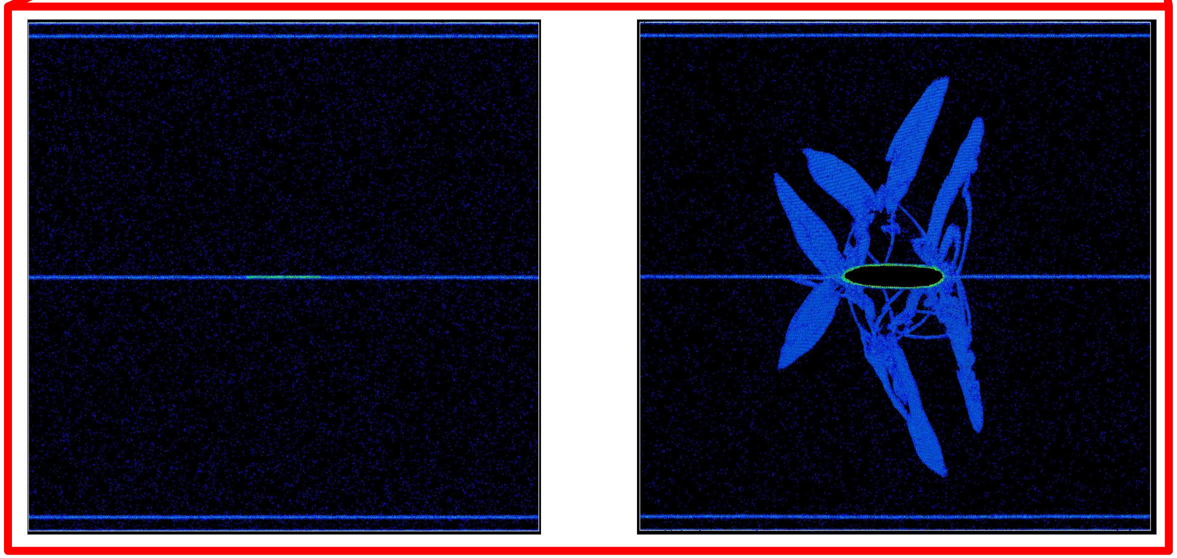

- **Avoids having to artificially impose a boundary velocity**

Simulating steady-state fracture

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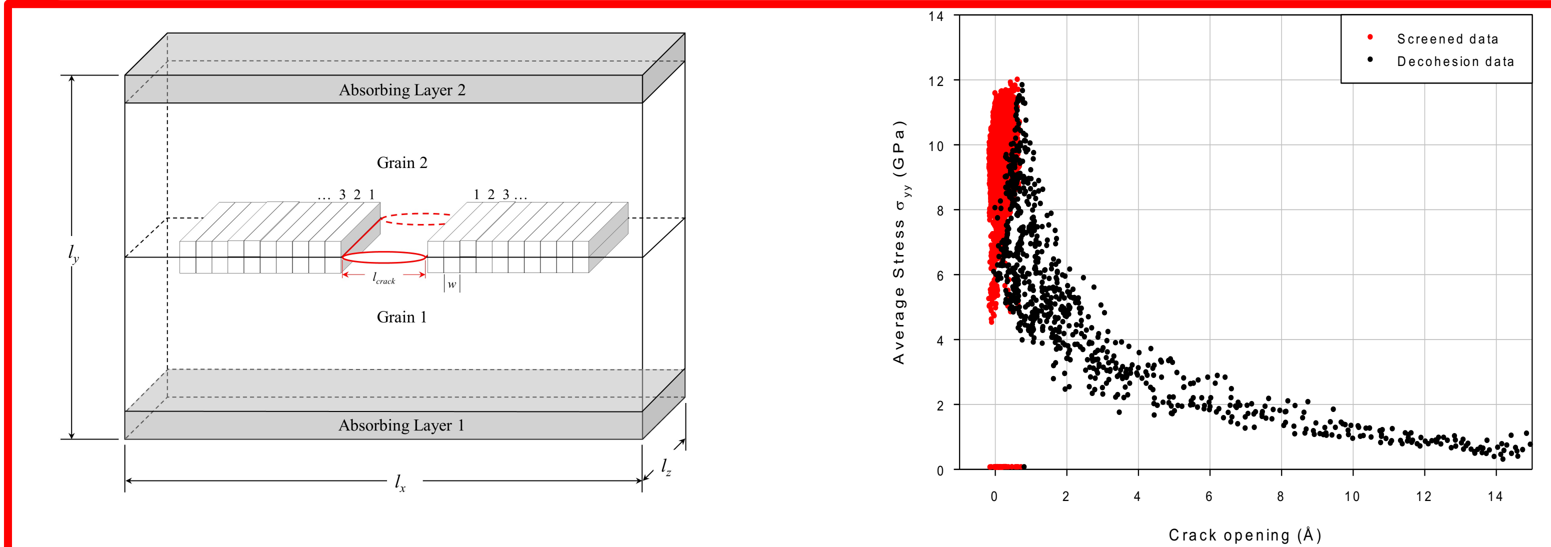

- **Statistical mechanics rather than a deterministic approach**

Mechanistically similar fracture behavior

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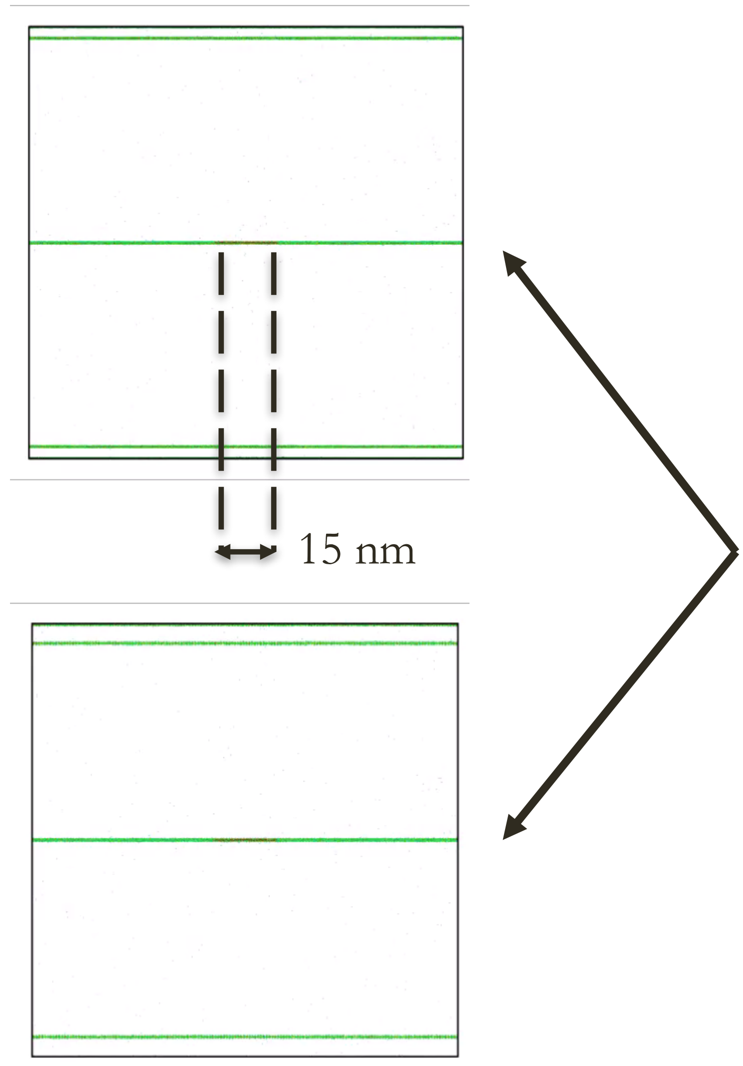
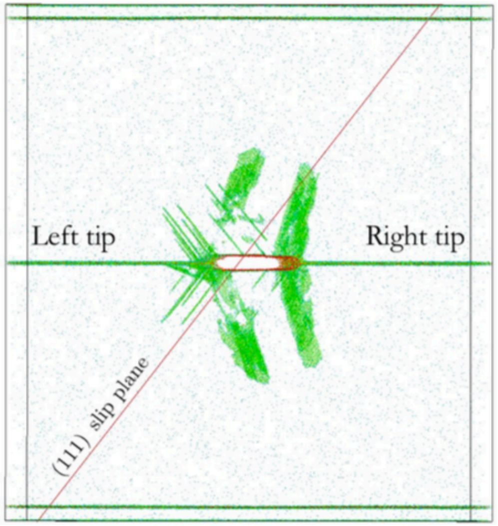
Crack propagation:
{213} STGB + 0 H/nm^2



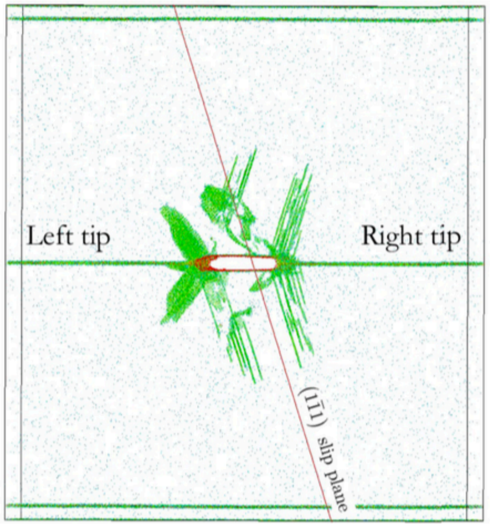
Crack propagation:
{415} STGB + 0 H/nm^2

Plasticity similar for both {213} and {415} as generally expected from Schmid Factor

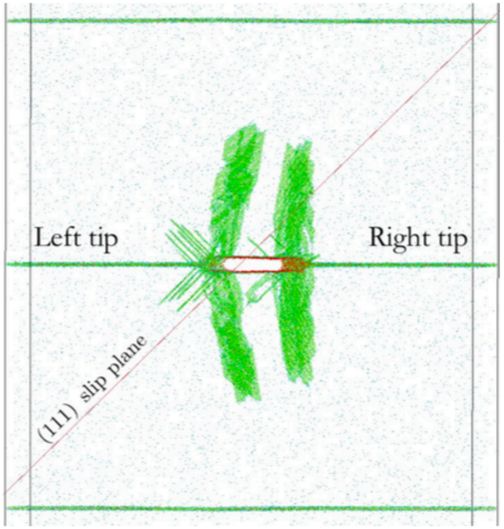
Mechanistically similar fracture behavior



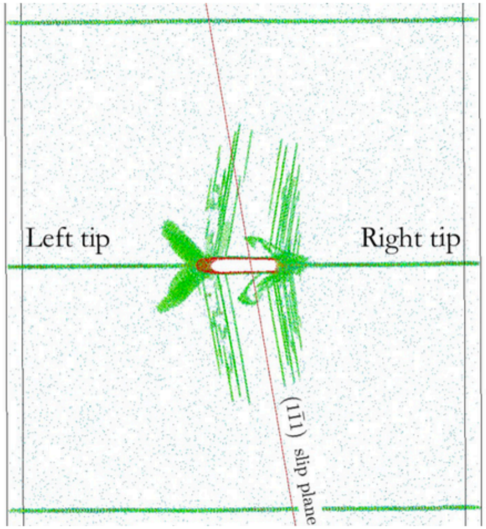
(a) {213} grain boundary:(111) slip plane



(b) {213} grain boundary: (1$\bar{1}$1) slip plane



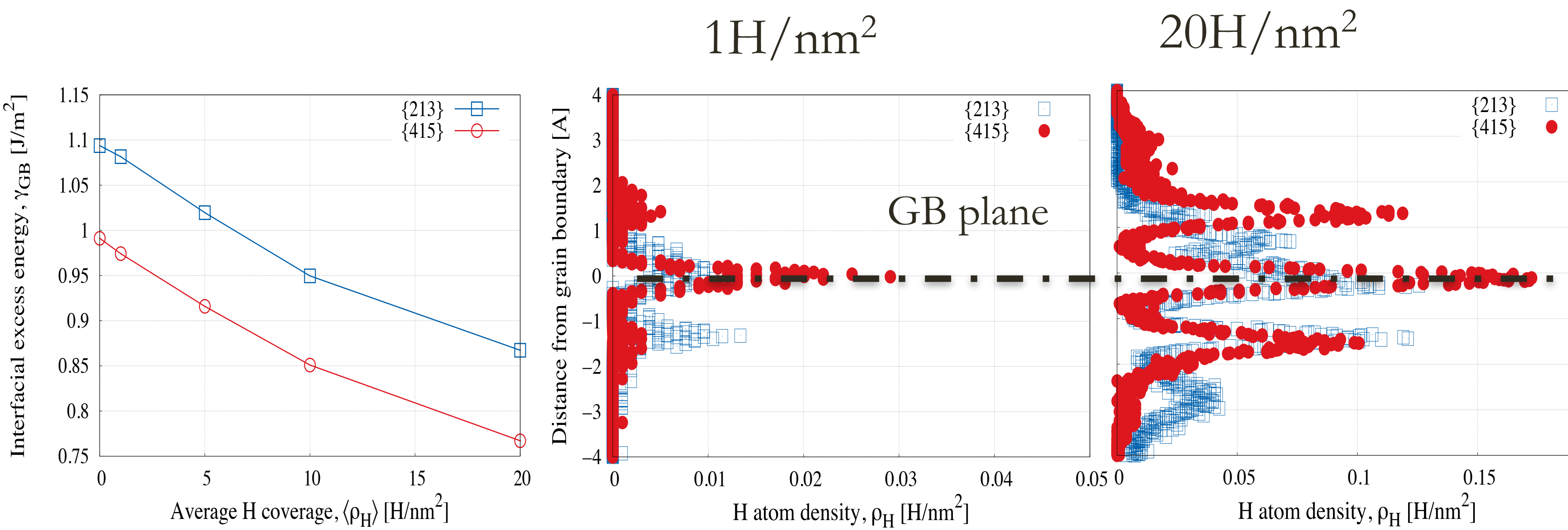
(c) {415} grain boundary: (111) slip plane



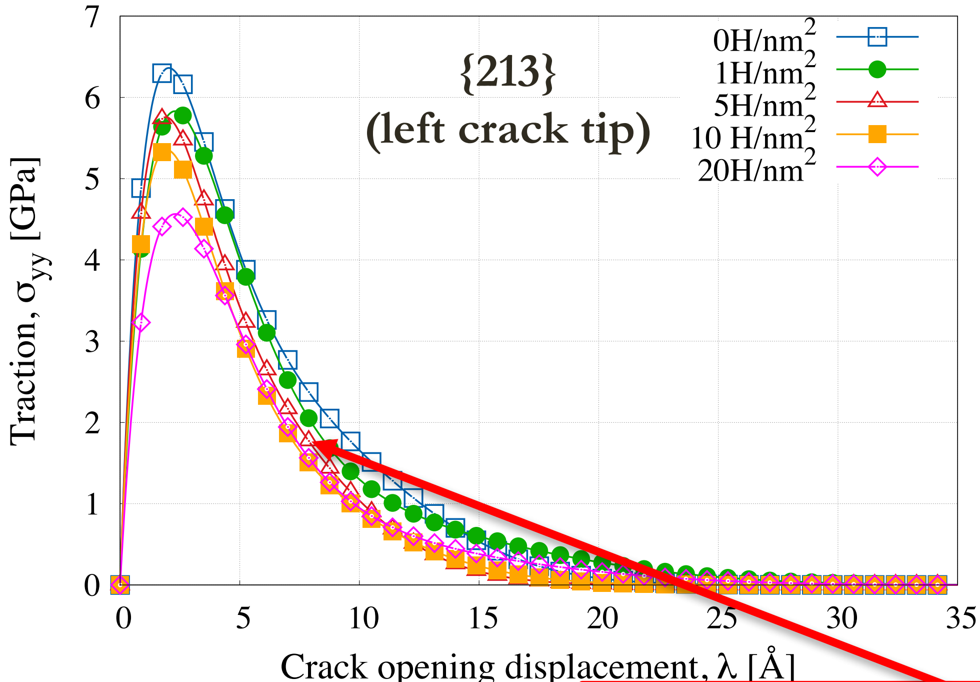
(d) {415} grain boundary: (1$\bar{1}$1) slip plane

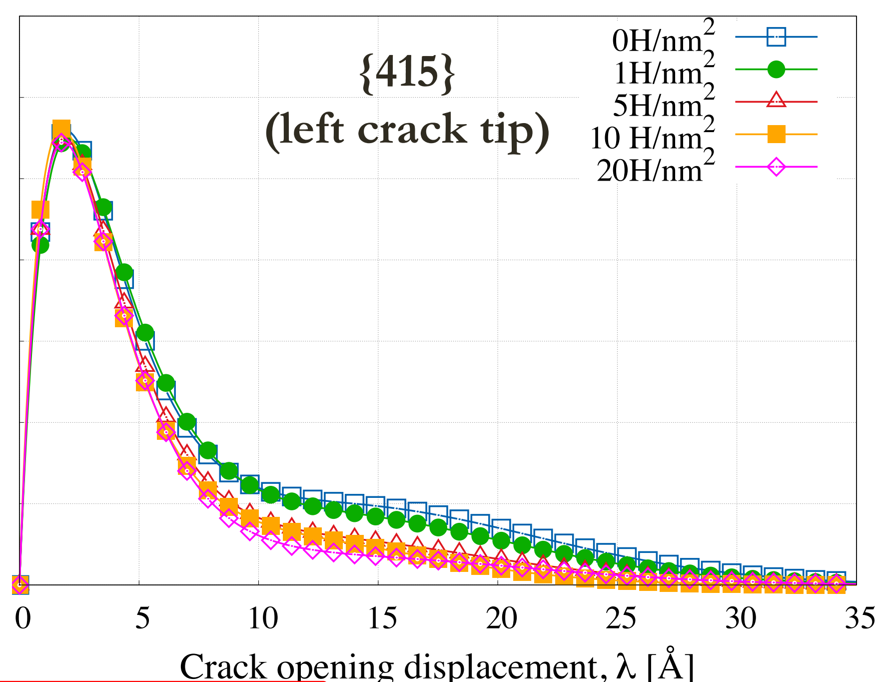
Using H segregation at GB as a surrogate for change in interfacial structure

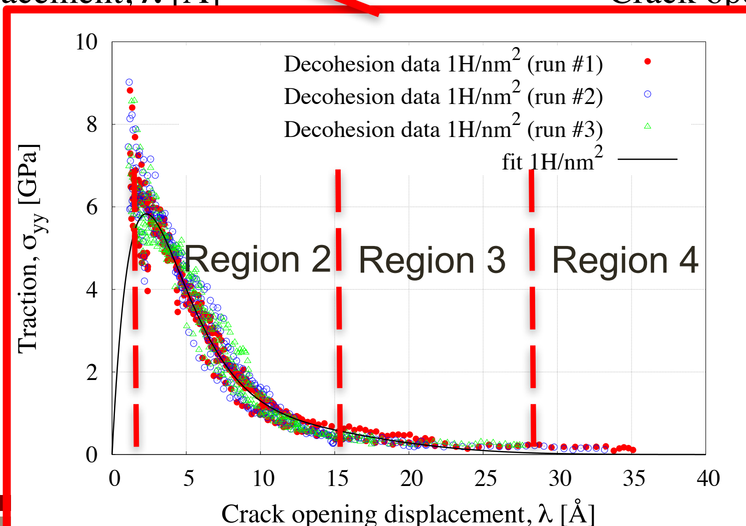
$$\Gamma = \frac{1}{A}\left[\sum_{N_{\mathrm{Ni}}}\left(E_{N_{\mathrm{Ni}}} - E^{\mathrm{bulk}}_{N_{\mathrm{Ni}}}\right) + \sum_{N_{\mathrm{H}}}\left(E_{N_{\mathrm{H}}} - E^{\mathrm{bulk}}_{N_{\mathrm{H}}}\right)\right]$$

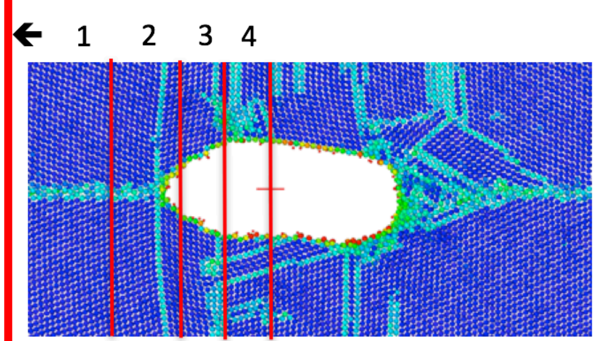


Isolating the role of the interface (1/2)

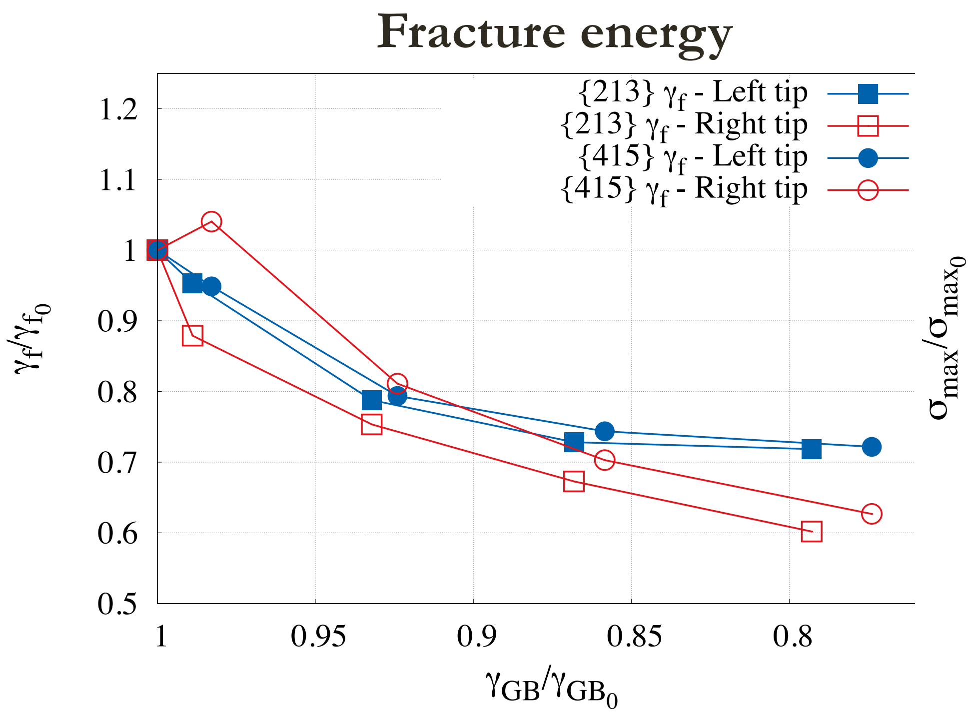


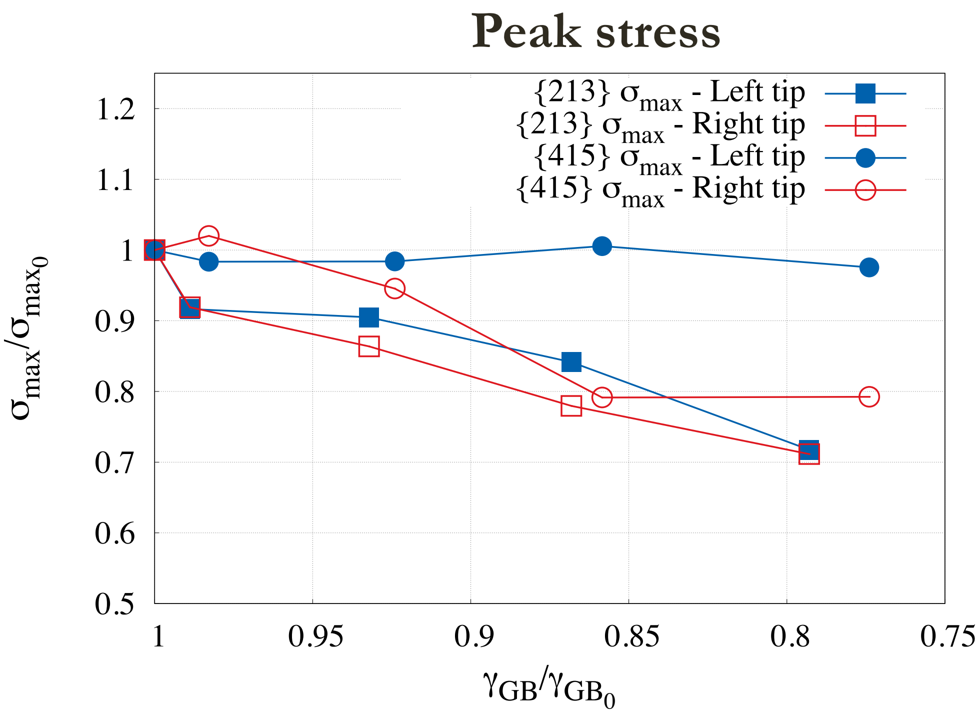






Isolating the role of the interface (2/2)

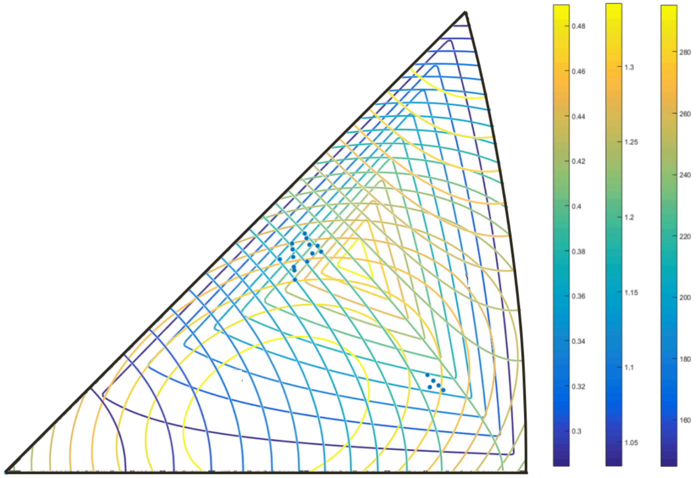


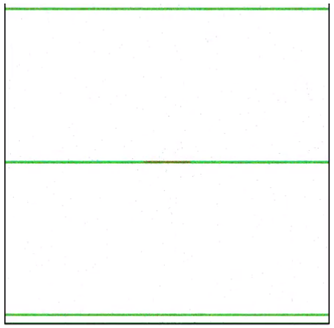


- In this example, structure of interface directly influence driving force for crack propagation!

Methodology to isolate role of GB structure

- Pathway for **identifying general GB predisposition** to resist fracture
  - Create sets of GBs using **isocurves associated with identical lattice properties** (E, μ^{α}, R_{μ})
  - Enable identification of **structure-property relationships**
  - High-throughput simulations underway





[Dingreville, Aksoy and Spearot, in press Sci. Reports, 2017]

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